Jan Delaval please

7/24/16

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABIHA QAZI (STIC) Examiner #: 74141 Date: 8/15/02

Art Unit: 1616 Phone Number 30 5-3910 Serial Number: 10/053505

Mail Box and Bldg/Room Location: 2019, CM1 3B07 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Bio available Prodrugs of Androgenic Steroids and related products.

Inventors (please provide full names): William J. Roberts

Earliest Priority Filing Date: 1/16/2002

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for

1) 4-Androstenediol Ethyl Carbonate diester. Monoester

2) "

3) 4-Androstenediol.

4) estr-4-ene-3,17 diol

5) as Compds of Cls. 3–6 & Cl 1

Please see attached sheets

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

Thank you.

****

STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher: Jan	NA Sequence (#)		STN	✓
Searcher Phone #: 4498	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	✓	Questel/Orbit	
Date Searcher Picked Up: 8/19/02	Bibliographic		Dr.Link	
Date Completed: 8/19/02	Litigation		Lexis/Nexis	
Searcher Prep & Review Time:	Fulltext		Sequence Systems	
Clerical Prep Time: 20	Patent Family		WWW/Internet	
Online Time: +50	Other		Other (specify)	

PTO-1590 (8-01)

10/053,505

WHAT IS CLAIMED IS:

1. A compound for increasing the concentration of a parent androgen in a subject in vivo, the parent androgen having a skeletal structure including a 4 position and a 17 position and the parent androgen further having a 17β-hydroxy group comprising a 17β-hydroxy oxygen appended to the 17 position and a 17β-hydroxy hydrogen appended to the 17β-hydroxy oxygen, the compound comprising:

a substrate having the skeletal structure of the parent androgen comprising a 4 position and a 17 position corresponding to the 4 and 17 positions respectively of the parent androgen, the substrate comprising a carbon-carbon double bond at the 4 position, the skeletal structure of the parent androgen embodied in the substrate being selected from the group consisting of androst-4-ene-3α,17β-diol, androst-4-ene-3β,17β-diol, and mixtures thereof; and

a promoiety appended to the 17β-hydroxy oxygen of the substrate as a substitute for the hydroxy hydrogen of the parent androgen, the promoiety comprising an alkylcarbonate ester.

2. A compound as set forth in claim 1, wherein the alkylcarbonate ester has an alkyl chain length of less than 12.

3. A compound as set forth in claim 1, wherein the compound comprises androst-4-ene-3,17β-diol 17β-alkylcarbonate.

4. A compound as set forth in claim 1, wherein the compound comprises androst-4-ene-3,17β-diol 17β-ethylcarbonate.

5. A compound as set forth in claim 1, wherein the compound comprises androst-4-ene-3,17β-diol 3,17β-di(alkylcarbonate).

6. A compound as set forth in claim 1, wherein the compound comprises androst-4-ene-3,17β-diol 3,17β-di(ethylcarbonate). $C_{25}H_{38}O_6$ L63

7. A compound as set forth in claim 1, further including a carrier.

8. A compound as set forth in claim 1, wherein the carrier comprises a solid carrier.

9. A compound as set forth in claim 1, wherein the carrier comprises a liquid carrier.

10. A compound as set forth in claim 1, wherein the carrier comprises a semi-solid carrier.

11. A compound for increasing the concentration of a parent androgen in a subject in vivo, the parent androgen having a skeletal structure including a 4 position and a 17 position and the parent androgen further having a 17β-hydroxy group comprising a 17β-hydroxy oxygen appended to the 17 position and a 17β-hydroxy hydrogen appended to the 17β-hydroxy oxygen, the compound comprising:

a substrate having the skeletal structure of the parent androgen comprising a 4 position and a 17 position corresponding to the 4 and 17 positions respectively of the parent androgen, the substrate comprising a carbon-carbon double bond at the 4 position, the skeletal structure of the parent androgen embodied in the substrate

being selected from the group consisting of estr-4-ene-3α,17β-diol, estr-4-ene-3β,17β-diol and mixtures thereof; and

a promoiety appended to the 17β-hydroxy oxygen of the substrate as a substitute for the hydroxy hydrogen of the parent androgen, the promoiety comprising an alkylcarbonate ester.

12. A compound as set forth in claim 11, wherein the alkylcarbonate ester has an alkyl chain length of less than 12.

13. A compound as set forth in claim 11, wherein the compound comprises estr-4-ene-3,17β-diol 17β-alkylcarbonate.

14. A compound as set forth in claim 11, wherein the compound comprises estr-4-ene-3,17β-diol 17β-ethylcarbonate.

15. A compound as set forth in claim 11, wherein the compound comprises estr-4-ene-3,17β-diol 3,17β-di(alkylcarbonate).

16. A compound as set forth in claim 11, wherein the compound comprises estr-4-ene-3,17β-diol 3,17β-di(ethylcarbonate).

17. A compound as set forth in claim 11, further including a carrier.

18. A compound as set forth in claim 11, wherein the carrier comprises a solid carrier.

19. A compound as set forth in claim 11, wherein the carrier comprises a liquid carrier.

20. A compound as set forth in claim 11, wherein the carrier comprises a semi-solid carrier.

21. A method for increasing the concentration of a parent androgen in a subject in vivo, the parent androgen having a skeletal structure including a 4 position and a 17 position and the parent androgen further having a 17β-hydroxy group comprising a 17β-hydroxy oxygen appended to the 17 position and a 17β-hydroxy hydrogen appended to the 17β-hydroxy oxygen, the method comprising:

administering to the subject a compound comprising a substrate and a promoiety, the substrate having the skeletal structure of the parent androgen comprising a 4 position and a 17 position corresponding to the 4 and 17 positions respectively of the parent androgen, and the substrate comprising a carbon-carbon double bond at the 4 position, the skeletal structure of the parent androgen embodied in the substrate being selected from the group consisting of androst-4-ene-3α,17β-diol, androst-4-ene-3β,17β-diol, and mixtures thereof, the promoiety being appended to the 17β-hydroxy oxygen of the substrate as a substitute for the 17β-hydroxy hydrogen of the parent androgen, the promoiety comprising an alkylcarbonate ester; and

converting the compound in vivo into the parent androgen.

22. A method as set forth in claim 21, wherein the subject is a human being and the in vivo conversion comprises converting the compound into the parent androgen in vivo within the human being.

40. A method for increasing the concentration of a parent androgen in a subject in vivo, the parent androgen having a skeletal structure including a 4 position and a 17 position and the parent androgen further having a 17β-hydroxy group comprising a 17β-hydroxy oxygen appended to the 17 position and a 17β-hydroxy hydrogen appended to the 17β-hydroxy oxygen, the method comprising:

administering to the subject a compound comprising a substrate and a promoiety, the substrate having the skeletal structure of the parent androgen comprising a 4 position and a 17 position corresponding to the 4 and 17 positions respectively of the parent androgen, and the substrate comprising a carbon-carbon double bond at the 4 position, the skeletal structure of the parent androgen embodied in the substrate being selected from the group consisting of estr-4-ene-3α,17β-diol, estr-4-ene-3β,17β-diol, and mixtures thereof, the promoiety being appended to the 17β-hydroxy oxygen of the substrate as a substitute for the 17β-hydroxy hydrogen of the parent androgen, the promoiety comprising an alkylcarbonate ester; and

converting the compound in vivo into the parent androgen.

41. A method as set forth in claim 40, wherein the subject is a human being and the in vivo conversion comprises converting the compound into the parent androgen in vivo within the human being.

42. A method as set forth in claim 40, wherein the compound comprises estr-4-ene-3,17β-diol 17β-alkylcarbonate.

台州市兴业化工厂质检报告单

TAIZHOU XINGYE CHEMICAL FACTORY

CERTIFICATE OF ANALYSIS

Product Name 产品名称: 4-androstenediol Ethyl Carbonate（4-雄烯二醇碳酸乙酯）

Manufacture Date 生产日期: Dec. 29, 2001

Batch No 批号: 20011229 Quantity 数量: 10kg

Packing 包装: 5kg/Tin Expiry Date 有效期: Dec. 29, 2003

Description 性状: white crystalline powder 白色结晶性粉末.

Tests 测试	Results 结果	Limits 限度
Melting point 熔点:	99.0-105.0℃	≥90℃
Loss on drying 干燥失重:	0.32%	≤0.5%
Residue on ignition 灼烧残渣:	0.01%	≤0.1%
Heavy metals 重金属:	complies	≤20PPM
Assay 含量:		
4-Androstenediol Ethyl Carbonate (Diester) 双酯		
	Complies	≥90%
4-Androstenediol Ethyl Carbonate (Monoester) 单酯		
	Complies	≤10%
4-Androstenediol Base 游离碱	Complies	≤1%

Conclusion: The specification conforms to the enterprise standard.

结论: 本品符合企业标准.

台州市兴业化工厂 质检科

*: Assay is performed by TLC test. 含量采用薄层色谱法测定

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FILE 'REGISTRY' ENTERED AT 15:32:35 ON 19 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:   18 AUG 2002  HIGHEST RN 444143-77-5
DICTIONARY FILE UPDATES:  18 AUG 2002  HIGHEST RN 444143-77-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Calculated physical property data is now available.  See HELP PROPERTIES
for more information.  See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d ide can tot l30

L30  ANSWER 1 OF 8  REGISTRY  COPYRIGHT 2002 ACS
RN   109715-20-0  REGISTRY
CN   Estr-4-ene-3,17-diol (6CI, 9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C18 H28 O2
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LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER
         (*File contains numerically searchable property data)

Absolute stereochemistry.
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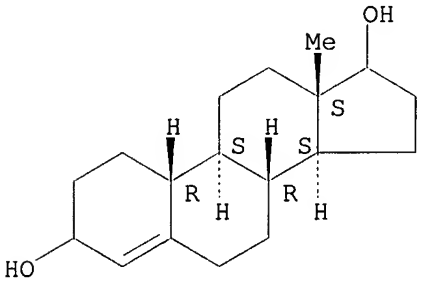


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REFERENCE   2:  135:299653

REFERENCE   3:  135:256352

REFERENCE   4:  135:252099

REFERENCE   5:  112:177410
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CM1 1E07 – 703-308-4498
jan.delaval@uspto.gov

L30 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 94424-29-0 REGISTRY
CN **Estr-4-ene-3,17-diol, (17.beta.)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estr-4-ene-3,17.beta.-diol (7CI)
FS STEREOSEARCH
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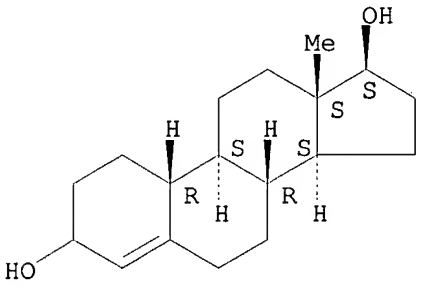
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.



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REFERENCE 1: 136:247403

REFERENCE 2: 134:280349

REFERENCE 3: 133:192756

REFERENCE 4: 131:281019

L30 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 81176-75-2 REGISTRY
CN **Androst-4-ene-3,17-diol, (17.beta.)- (9CI)** (CA INDEX NAME)
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MF C19 H30 O2
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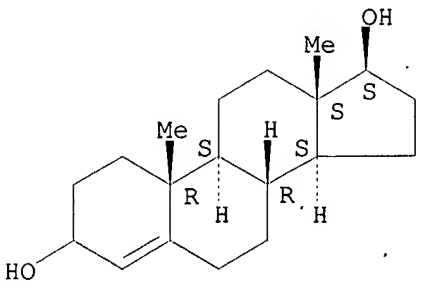
(*File contains numerically searchable property data)

Absolute stereochemistry.



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REFERENCE 2: 119:250227

REFERENCE 3: 96:162253

L30 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN 35950-87-9 REGISTRY
CN **Estr-4-ene-3,17-diol, (3.alpha.,17.beta.)- (9CI)** (CA INDEX NAME)
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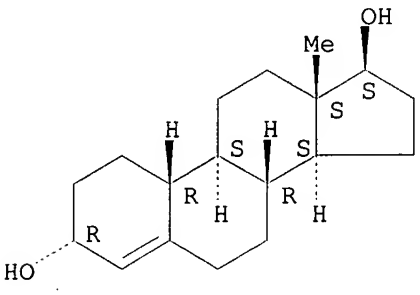
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



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REFERENCE 2: 125:248219

REFERENCE 3: 76:141147

L30 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN **19793-20-5** REGISTRY
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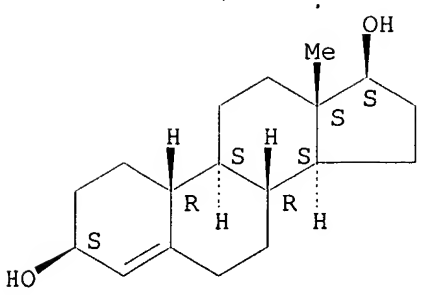
OTHER NAMES:
CN .DELTA.4-Estrene-3.beta.,17.beta.-diol
CN Bolandiol
FS STEREOSEARCH
MF C18 H28 O2
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CHEMCATS, CHEMLIST, DDFU, DRUGU, MRCK*, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO

Absolute stereochemistry.



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21 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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REFERENCE 2: 136:241867

REFERENCE 3: 136:11113

REFERENCE 4: 135:268444

REFERENCE 5: 135:268442

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REFERENCE 7: 132:31279

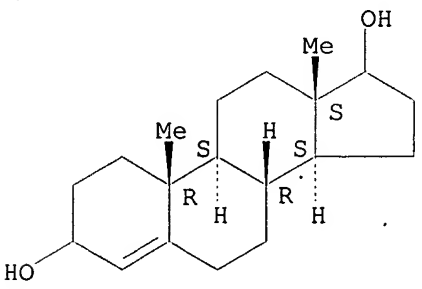
REFERENCE 8: 130:200924

REFERENCE 9: 125:248219

REFERENCE 10: 123:340530

L30 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN **17218-62-1** REGISTRY
CN **Androst-4-ene-3,17-diol (7CI, 8CI, 9CI)** (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H30 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



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REFERENCE 1: 136:330323

REFERENCE 2: 136:123403

REFERENCE 3: 135:308592

REFERENCE 4: 113:165578

REFERENCE 5: 109:109870

REFERENCE 6: 101:7047

REFERENCE 7: 99:52583

REFERENCE 8: 87:115429

REFERENCE 9: 77:58282

REFERENCE 10: 67:105640

L30 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN **1852-61-5** REGISTRY
CN **Androst-4-ene-3,17-diol, (3.alpha.,17.beta.)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Androst-4-ene-3.alpha.,17.beta.-diol (7CI, 8CI)
OTHER NAMES:
CN 3.alpha.,17.beta.-Dihydroxyandrost-4-ene
FS STEREOSEARCH
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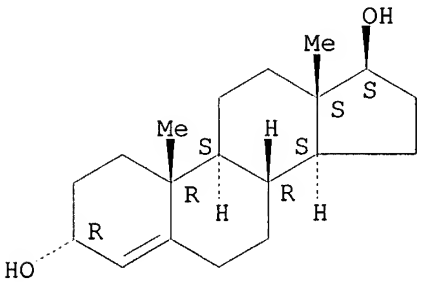
Absolute stereochemistry.



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7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:351500

REFERENCE 2: 130:218734

REFERENCE 3: 130:164199

REFERENCE 4: 126:171765

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REFERENCE 6: 120:164666

REFERENCE 7: 112:156719

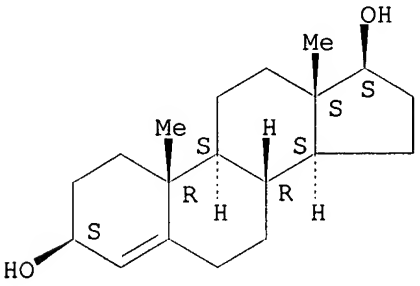
REFERENCE 8: 111:174513

REFERENCE 9: 110:189105

REFERENCE 10: 109:23183

L30 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2002 ACS
RN **1156-92-9** REGISTRY
CN **Androst-4-ene-3,17-diol, (3.beta.,17.beta.)- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Androst-4-ene-3.beta.,17.beta.-diol (7CI, 8CI)
OTHER NAMES:
CN .DELTA.4-Androstene-3.beta.,17.beta.-diol
CN 3.beta.,17.beta.-Dihydroxy-4-androstene
CN **4-Androstenediol**
FS STEREOSEARCH
MF C19 H30 O2
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CIN, CSCHEM, EMBASE, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



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29 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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REFERENCE 2: 136:304231

REFERENCE 3: 136:161484

REFERENCE 4: 136:11113

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REFERENCE 6: 135:268442

REFERENCE 7: 135:151866

REFERENCE 8: 135:112013

REFERENCE 9: 134:361828

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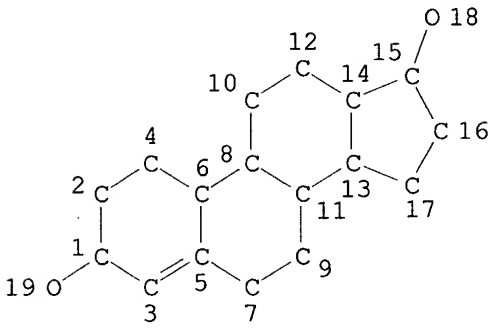

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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 19

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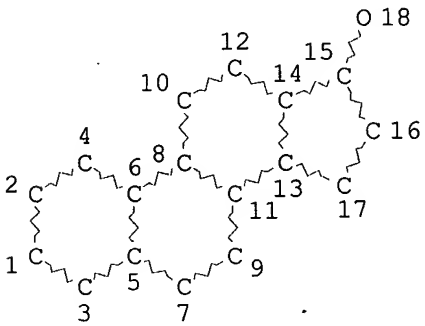

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 18

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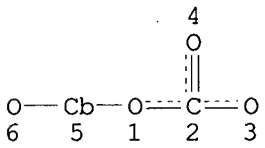

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
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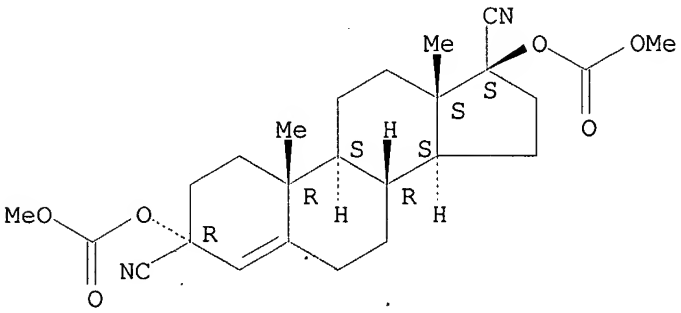
L70 4 SEA FILE=REGISTRY ABB=ON PLU=ON L69 NOT C27H36O4
L71 1 SEA FILE=REGISTRY ABB=ON PLU=ON L70 AND C25H38O6
L72 3 SEA FILE=REGISTRY ABB=ON PLU=ON L70 NOT L71
L73 2 SEA FILE=REGISTRY ABB=ON PLU=ON L72 NOT C6/ES
L74 3 SEA FILE=REGISTRY ABB=ON PLU=ON (L71 OR L73)

=> d l74 ide can tot

L74 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2002 ACS
RN 301522-32-7 REGISTRY
CN Androst-4-ene-3,17-dicarbonitrile, 3,17-bis[(methoxycarbonyl)oxy]-, (3.alpha.,17.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H32 N2 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:296008

L74 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2002 ACS
RN 301522-31-6 REGISTRY
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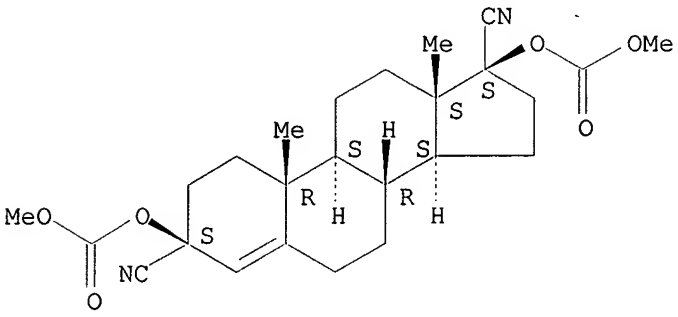
FS STEREOSEARCH
MF C25 H32 N2 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



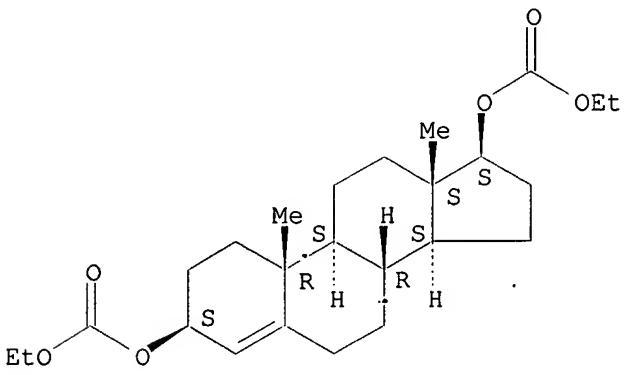
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:296008

L74 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2002 ACS
RN 10583-86-5 REGISTRY
CN Androst-4-ene-3.beta.,17.beta.-diol, bis(ethyl carbonate) (7CI, 8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C25 H38 O6**
LC STN Files: CAOLD

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his l74-

(FILE 'REGISTRY' ENTERED AT 15:10:35 ON 19 AUG 2002)
L74 3 S L71,L73
SAV L74 QAZI053A/A

FILE 'HCAOLD' ENTERED AT 15:31:15 ON 19 AUG 2002
L75 1 S L74
SEL AN
EDIT /AN /OREF

FILE 'HCAPLUS' ENTERED AT 15:31:53 ON 19 AUG 2002
L76 2 S E9
L77 1 S L76 NOT CASPI ?/AU
L78 1 S L74

FILE 'REGISTRY' ENTERED AT 15:32:35 ON 19 AUG 2002

=> fil hcaold
FILE 'HCAOLD' ENTERED AT 15:33:08 ON 19 AUG 2002

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

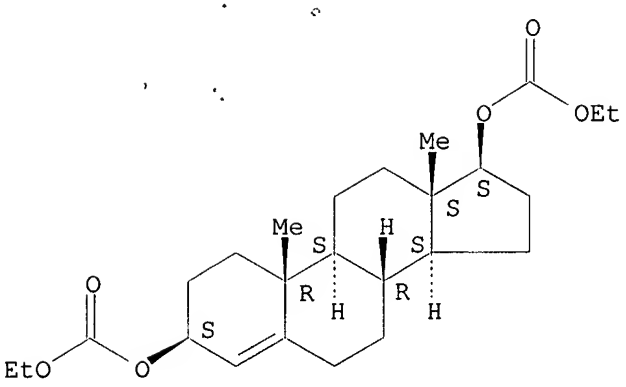
This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d l75 all hitstr

L75 ANSWER 1 OF 1 HCAOLD COPYRIGHT 2002 ACS
AN CA65:18648e CAOLD
TI neighboring-group participation on 3.beta.-acetate, -mixed carbonate, or -urethan groups in acid-catalyzed cleavage of 4.alpha.,5.alpha.-epoxysteroids
AU Julia, Sylvestre; Furer, B.
IT 747-90-0 1156-92-9 1852-61-5 1917-78-8 6564-48-3 10458-44-3
10459-14-0 10459-15-1 10459-16-2 10459-17-3 10459-18-4 10459-19-5
10459-20-8 10459-21-9 **10583-86-5** 10583-87-6 10583-88-7
10583-89-8 10587-46-9 10587-47-0 13001-01-9 13123-29-0 13262-58-3
13289-03-7 13289-04-8 13312-54-4 13381-18-5
IT **10583-86-5**
RN 10583-86-5 HCAOLD
CN Androst-4-ene-3.beta.,17.beta.-diol, bis(ethyl carbonate) (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 15:33:14 ON 19 AUG 2002

FILE COVERS 1907 - 19 Aug 2002 VOL 137 ISS 8
FILE LAST UPDATED: 18 Aug 2002 (20020818/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> d all l77

L77 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
AN 1966:499550 HCAPLUS
DN 65:99550
OREF 65:**18648e-h,18649a-h,18650a**
TI Neighboring-group participation of 3.beta.-acetate, -mixed carbonate, or -urethan groups in acid-catalyzed cleavage of 4.alpha.,5.alpha.epoxy steroids
AU Julia, Sylvestre; Furer, Beat
CS Ecole Natl. Super. Chim., Paris
SO Bull. Soc. Chim. France (1966), (3), 1106-14
DT Journal
LA French
CC 42 (Steroids)
GI For diagram(s), see printed CA Issue.
AB cf. CA 59, 10167b. Cleavage of 3.beta.,17.beta.-diacetoxy-

4.alpha.,5.alpha.epoxyandrostane (I) with BF3.Et2O in MeOH gave 17.beta.-acetoxyandrostane-3.beta.,4.beta.,5.alpha.-triol (II) presumably through hydrolysis of an orthoacetate intermediate. With 2N H2SO4 or BF3.Et2O in C6H6 I gave 4.beta.,17.beta.-diacetoxyandrostane-3.beta.,5.alpha.-diol (III) by Ac migration. BF3.Et2O (0.1 ml.) and 300 mg. I in 20 ml. MeOH kept at room temp. and H2O added after 2 hrs. gave 53% II, m. 215-17.degree. (Me2CO-ligroine), [.alpha.]D 3.8.degree. (c 0.33, CHCl3). I (3.7 g.) in 750 ml. Me2CO and 7.5 ml. 2N H2SO4 in 75 ml. H2O kept at room temp. and the Me2CO evapd. after 3 days gave 3 g. III, m. 228-30.degree. (Me2CO), [.alpha.]D 4.3.degree. (c 0.54, CHCl3). Similarly, 250 mg. I in 30 ml. C6H6 and 15 ml. Et2O and 0.5 ml. BF3.Et2O stirred at room temp. for 3 hrs. gave 34% III. III (100 mg.) in 2 ml. C5H5N treated with 1 ml. Ac2O and kept at room temp. overnight gave 55% 3.beta.,4.beta.,17.beta.-triacetoxyandrostan-5.alpha.-ol, m. 162-3.degree. (MeOH-H2O), [.alpha.]D -6.degree. (c 1.18, CHCl3). III (1.7 g.) in 500 ml. Et2O and 50 ml. tetrahydrofuran and 1 g. LiAlH4 refluxed for 2 hrs. and kept at room temp. overnight gave 75% androstane-3.beta.,4.beta.,5.alpha.,17.beta.-tetraol (IV), m. 265-8.degree. (MeOH), [.alpha.]D 11.degree. (c 0.2, EtOH). IV (500 mg.) and 5 ml. Ac2O in 5 ml. C5H5N kept at room temp. overnight gave 50% 3.beta.,17.beta.-diacetoxyandrostane-4.beta.,5.alpha.-diol (V), m. 205-7.degree. (Me2CO-MeOH), [.alpha.]D 3.6.degree. (c 0.32, CHCl3). Alternatively, 100 mg. 3.beta.,17.beta.-diacetoxy-4.beta.,5.beta. epoxyandrostane in 20 ml. Me2CO and 2 ml. H2O treated with 0.2 ml. 2N H2SO4 and the Me2CO evapd. after 3 days gave 72% V. Acid-catalyzed cleavage of 3.beta.-ethoxycarbonyloxy-4.alpha.,5.alpha.-epoxycholestane (VI) and 3.beta.,17.beta.-bis(ethoxycarbonyloxy)-4.alpha.,5.alpha.-epoxyandrostane (VII) gave the corresponding cyclic carbonates (VIII) through neighboring-group participation. A soln. of 4 g. 3.beta.-hydroxycholest-4-ene (IX) in 120 ml. C5H5N was treated with 12 ml. ethyl chloroformate at 0.degree., the mixt. poured onto ice after 12 hrs., and the ppt. washed with H2O to give 75-80% 3.beta.-ethoxycarbonyloxycholest-4-ene (X), m. 101-2.degree. (Me2CO-MeOH), [.alpha.]D 10.degree. (c 0.67, CHCl3). X (459 mg.) in 15 ml. Et2O treated with 340 mg. p-nitroperbenzoic acid in 3 ml. tetrahydrofuran, the mixt. dild. with Et2O after 24 hrs., washed with satd. Na2CO3 soln. and H2O, dried, and evapd. gave 70-75% VI, m. 106-7.degree. (Me2CO-MeOH), [.alpha.]D 45.degree. (c 1.1, CHCl3). Dropwise addn. of 0.7 ml. ethyl chloroformate to a soln. of 150 mg. 3.beta.hydroxy-4.alpha.,5.alpha.-epoxycholestane in 5 ml. C5H5N at room temp. gave 81% VI. A soln. of 475 mg. VI in 10 ml. tetrahydrofuran refluxed with 1.5 ml. 30% HClO4 for 6 hrs. gave 70% VIII (R = C8H17), m. 248-50.degree. (Me2CO-MeOH), [.alpha.]D 38.degree. (c 0.5, CHCl3). Similarly, 130 mg. VI in 6 ml. Me2CO heated at 30.degree. with 0.3 ml. 48% HBr soln. gave 86% VIII (R = C8H17) on addn. of H2O after 45 min. A soln. of 150 mg. cholestane-3.beta.,4.beta.,5.beta.-triol in 50 ml. CHCl3 and 3 ml. C5H5N treated with 75 ml. of a 20% soln. of COCl2 in toluene at 20.degree., satd. NaHCO3 soln. added after 48 hrs., the org. soln. washed with 2N HCl soln., NaHCO3 soln., and H2O, dried, and evapd. gave 67% VIII (R = C8H17). SOCl2 (1 ml.) added dropwise to 200 mg. VIII (R = C8H17) in 5 ml. C5H5N at 0.degree., the mixt. poured onto ice after 20 min., extd. with Et2O, the soln. washed with 2N H2SO4, satd. NaHCO3, and H2O gave 89% of the cyclic carbonate (XI), m. 164-5.degree. (Me2CO-MeOH), [.alpha.]D-24.degree. (c 0.2, CHCl3). Addn. of 50 ml. of a 20% soln. of COCl2 in toluene to 100 mg. cholest-5-ene-3.beta.,4.beta.-diol and the mixt. worked up after 2 days at 20.degree. also gave XI. Epoxidn. of IX with a soln. of HClO4 in Et2O at 0.degree. gave a crude product, which was treated with 1 ml. ethyl chloroformate in 10 ml. C5H5N. Chromatography of the product on neutral alumina and elution with 10% C6H6-petroleum ether gave 40.degree.50% 3.beta.-ethoxycarbonyloxy-4.beta.,5.beta.-epoxycholestane (XII), m. 100-1.degree. (Me2CO), [.alpha.]D 28.degree. (c 0.17, CHCl3). A soln. of 237 mg. XII in 5 ml. tetrahydrofuran treated with 0.7 ml. of 30% soln. of HClO4 for 4 hrs., the mixt. dild. with Et2O, washed with H2O, dried, and evapd. gave 80-90% 3.beta.-

ethoxycarbonyloxycholestane-4.beta.,5.alpha.-diol (XIII), m. 156-7.degree. (Me2CO), [.alpha.]D 14.degree. (c 0.6, CHCl3). Alternatively, treatment of 150 mg. cholestane-3.beta.,4.beta.,5.alpha.-triol in 5 ml. C5H5N with 0.7 ml. ethyl chloroformate gave 88% XIII. Dropwise addn. of 3 ml. ethyl chloroformate to 700 mg. androst-4-ene-3.beta.,17.beta.-diol in 20 ml. C5H5N at 0.degree. gave 90% 3.beta.,17.beta.-bis(ethoxycarbonyloxy)-androst-4-ene (XIV), m. 105-6.degree. (ligroine), [.alpha.]D 3.degree. (c 0.68, CHCl3). Epoxidn. of 750 mg. XIV in 25 ml. Et2O with 560 mg. p-nitroperbenzoic acid in 5 ml. tetrahydrofuran gave 66% VII, m. 123-4.degree. (ligroine), [.alpha.]D 32.degree. (c 0.87, CHCl3). A soln. of 200 mg. VII in 5 ml. tetrahydrofuran refluxed with 0.8 ml. 30% HClO4 for 8 hrs. gave 75% VIII (R = OCO2Et), m. 204-5.degree., [.alpha.]D 17.degree. (c 0.23, CHCl3). Dropwise addn. of 0.6 ml. ethyl chloroformate to 150 mg. 3.beta.,17.beta.-dihydroxy-4.beta.,5.beta.-epoxyandrostane in 4 ml. C5H5N at 0.degree. and the mixt. poured into ice after 12 hrs. gave 60% 3.beta.,17.beta.-bis(ethoxycarbonyloxy)-4.beta.,5.beta.-epoxyandrostane (XV), m. 89-91.degree. (Me2CO), [.alpha.]D 33.degree. (c 0.56, CHCl3). A soln. of 120 mg. androstane-3.beta.,4.beta.,5.alpha.,17.beta.-tetraol in 3 ml. C5H5N treated with 0.5 ml. ethyl chloroformate gave 75% 3.beta.,17.beta.-bis(ethoxycarbonyloxy)androstane-4.beta.,5.alpha.-diol (XVI), m. 182-3.degree. [.alpha.]D 0.degree. (c 0.73, CHCl3). Cleavage of 50 mg. XV in 2 ml. tetrahydrofuran with 0.3 ml. HClO4 at room temp. for 4 hrs. also gave XVI. Acidcatalyzed cleavage of 3.beta.-phenylcarbamoyloxy-4.alpha.,5.alpha.-epoxycholestane (XVII) gave the cyclic carbonate VIII (R = C8H17) through neighboring-group participation, whereas 3.beta.-phenylcarbamoyloxy 4-methyl-4.alpha.,5.alpha.-epoxycholestane (XVIII) gave only 3.beta.-phenylcarbamoyloxy-4.alpha.-methylcholestane-4.beta.,5.alpha.-diol (XIX), by normal ring-opening. Cholest-4-en-3-ol (1 g.) and 1 ml. phenyl isocyanate heated together for 5 min. at 100.degree. gave 65.degree. 3.beta.-phenylcarbamoyloxycholest-4-ene (XX), m. 119-20.degree. (ligroine), [.alpha.]D 5.degree. (c 0.3, CHCl3). Epoxidn. of 506 mg. XX in 15 ml. Et2O with 400 mg. p-nitroperbenzoic acid in 4 ml. tetrahydrofuran for 24 hrs. gave 67% XVII, m. 156-7.degree., [.alpha.]D 38.degree. (c 0.19, CHCl3). Alternatively, treatment of 100 mg. 4.alpha.,5.alpha.-epoxycholestan-3.beta.-ol with 0.1 ml. phenyl isocyanate yielded 69% XVII. A soln. of 130 mg. XVII in 6 ml. Me2CO treated with 0.3 ml. 48% HBr at 30.degree., H2O added after 1 hr., the ppt. washed with H2O and dried gave 86% VIII (R = C8H17). A soln. of 130 mg. 3.beta.-phenylcarbamoyloxycholest-4-ene in 6 ml. Me2CO treated with 0.3 ml. 48% HBr and H2O added after 1 hr. gave 90% cholesta-3,5-diene, m. 76-7.degree. (Me2CO). Treatment of 100 mg. 3.beta.-phenylcarbamoyloxy-4-methylcholest-4-ene in 10 ml. Me2CO with 0.3 ml. HBr gave 95% 4-methylcholesta-3,5-diene, m. 74-5.degree. (Me2CO). Epoxidn. of 500 mg. 3.beta.-phenylcarbamoyloxy-4-methylcholest-4-ene in 15 ml. Et2O with 400 mg. p-nitroperbenzoic acid in 4 ml. tetrahydrofuran for 36 hrs. gave 08% XVIII, m. 204-5.degree. [.alpha.]D 50.degree. (C 0.38, CHCl3). Alternatively, 4.alpha.,5.alpha.-epoxy-4.beta.methylcholestan-3.beta.-ol treated with phenyl isocyanate yielded XVIII. A soln. of 200 mg. XVIII in 4 ml. tetrahydrofuran treated with 0.6 ml. 30% HClO4, H2O added after 4 hrs., the mixt. extd. with Et2O, the ext. washed with H2O, dried, and evapd. gave XIX, m. 199-201.degree. (Me2CO). Treatment of 4.alpha.-methylcholestane-3.beta.,4.beta.,5.alpha.-triol with phenyl isocyanate also gave XIX. A soln. of 4.2 g. 3.beta.-acetoxycholest-4-ene in dioxane treated with N-bromosuccinimide and dil. HClO4 gave 2.5 g. 4.beta.-acetoxy-5.alpha.-bromocholestan-3.beta.-ol (XXI), m. 145.degree. (Me2CO). Cyclization of XXI with KOH in MeOH and extn. with Et2O gave 1.88 g. 4.beta.,5.beta.-epoxycholestan-3.beta.-ol which was treated with 0.9 ml. phenyl isocyanate for 15 min. at 100.degree., the mixt. dild. with anhyd. ligroine and kept for 3 days at room temp. to give 1.42 g. 3.beta.-phenylcarbamoyloxy-4.beta.,5.beta.-epoxycholestane (XXII), m. 124-6.degree. (ligroine), [.alpha.]D -17.degree. (c 0.5, CHCl3). A soln. of 200 mg. XXII in 7 ml. tetrahydrofuran treated with 0.5 ml. 30% HClO4,

and H2O added after 5 hrs. gave 3.beta.-phenylcarbamoyloxycholestane-4.beta.,5.alpha.-diol, m. 234-6.degree. (Me2CO), [.alpha.]D 6.degree. (c 0.4, CHCl3).

=> d all hitstr l78

L78 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
AN 2000:559567 HCAPLUS
DN 133:296008
TI O-Methoxycarbonyl Cyanohydrin as a New Protective Group for Carbonyls
AU Berthiaume, D.; Poirier, D.
CS Oncology and Molecular Endocrinology Research Center, Medicinal Chemistry Division, Laval University Medical Center (CHUL), QC, G1V 4G2, Can.
SO Tetrahedron (2000), 56(33), 5995-6003
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 133:296008
AB O-Methoxycarbonyl cyanohydrin, a new protective group of carbonyls, was prepd. in high yields by an efficient one-step procedure using Me cyanoformate and a secondary alkylamine at room temp. The authors report efficient methods for the formation and cleavage of the protective group. Also, the ability of different types of carbonyls to be protected and the protective group's behavior under different chem. conditions were studied.
ST methoxycarbonyl cyanohydrin protective group carbonyl compd
IT Protective groups
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)
IT Carbonyl compounds (organic), preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)
IT 63-05-8, Androst-4-ene-3,17-dione 100-50-5, 3-Cyclohexene-1-carboxaldehyde 100-52-7, Benzaldehyde, reactions 104-53-0, Benzenepropanal 120-44-5 123-19-3, 4-Heptanone 502-49-8, Cyclooctanone 930-68-7, 2-Cyclohexen-1-one 1078-19-9 1624-62-0 5949-05-3 17640-15-2 33892-75-0 57711-43-0 58701-44-3 160840-44-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)
IT 246160-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)
IT 66867-29-6P 203510-62-7P 246160-21-4P 246160-22-5P 246160-23-6P 246160-25-8P 246160-26-9P 301522-28-1P 301522-29-2P 301522-30-5P **301522-31-6P 301522-32-7P** 301522-33-8P 301522-34-9P 301522-35-0P 301522-36-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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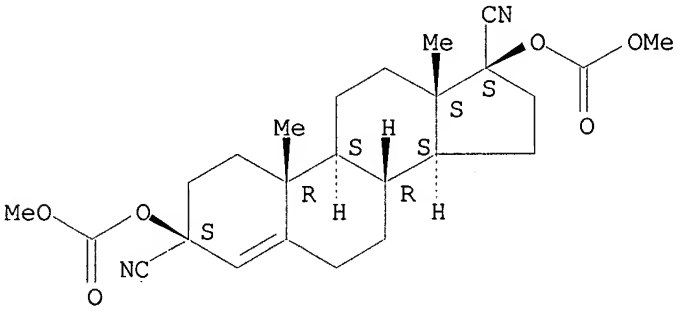
(26) Uff, B; Synth Commun 1978, V8, P163 HCAPLUS

IT **301522-31-6P 301522-32-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(use of O-methoxycarbonyl cyanohydrin as a protective group for carbonyls)

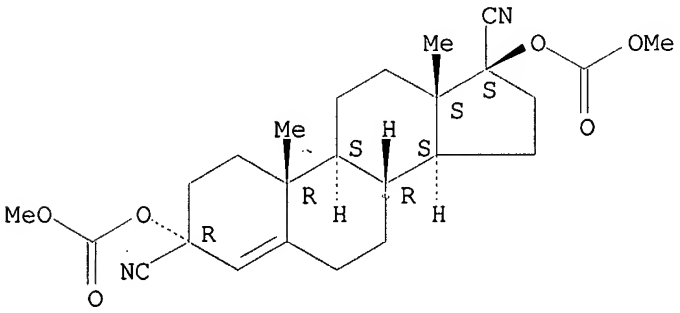
RN 301522-31-6 HCAPLUS
CN Androst-4-ene-3,17-dicarbonitrile, 3,17-bis[(methoxycarbonyl)oxy]-, (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 301522-32-7 HCAPLUS
CN Androst-4-ene-3,17-dicarbonitrile, 3,17-bis[(methoxycarbonyl)oxy]-, (3.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L1          105 S E3,E21-E23
L2           67 S E78,E93-E96
L3            2 S E127,E129
L4          174 S L1-L3
L5            0 S L4 AND STEROID?/SC,SX,CW
L6          216 S ESTR 4 ENE
L7         1720 S ANDROST 4 ENE
L8         1904 S L6,L7
L9          231 S L8 AND (17BETA OR 17B OR 17()(B OR BETA))()DIOL
L10          89 S L8 AND 17 DIOL
L11         304 S L9,L10
L12         221 S L11 AND (3A OR 3B OR 3ALPHA OR 3BETA OR 3()(ALPHA OR BETA OR
L13         253 S L11 AND 3 17
L14         296 S L12,L13
L15          58 S L14 NOT 17 DIONE

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L17           1 S 1852-61-5
L18           1 S 19793-20-5
L19           1 S 1156-92-9
               E ESTR-4-ENE-3,17-DIOL/CN
L20           1 S E3
L21           1 S E5
L22           1 S E7
               E ANDROST-4-ENE-3,17-DIOL/CN
L23           1 S E3
L24           1 S E6
L25           1 S E8
L26           1 S E4
               E ESTR-4-ENE-3,17-DIOL/CN
L27           1 S E4
L28           8 S L16-L27
               E 4-ANDROSTENEDIOL/CN
L29           1 S E3
L30           8 S L28,L29
               SEL RN
L31           0 S E1-E8/CRN

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L34           0 S L32 AND ?ALKYLCARBONATE?
L35           0 S L32 AND ?ETHYLCARBONATE?
L36           0 S L32 AND (TAIZHOU? OR XINGY?)/PA,CS
L37         222 S (TAIZHOU? OR XINGY?)/PA,CS
L38           0 S L37 AND STEROID?/SC,SX
L39           0 S L37 AND STEROID?/CW
L40           0 S L32 AND L4

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     FILE 'REGISTRY' ENTERED AT 15:10:25 ON 19 AUG 2002
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L41          SEL L32 1- RN :    2505 TERMS
                SET SMARTSELECT OFF

     FILE 'REGISTRY' ENTERED AT 15:10:35 ON 19 AUG 2002
L42         2503 S L41
L43         1452 S L42 AND C5-C6-C6-C6/ES
L44           63 S L43 AND ESTER
L45           53 S L44 NOT N/ELS
L46           29 S L45 AND (ANDROS? OR ESTR?)
L47        29673 S 4432.3.20/RID
L48          423 S L42 AND L47
L49           26 S L48 AND ESTER
L50               STR
L51       229631 S 4432/RID
L52           46 S L50 SAM SUB=L51
L53               STR L50
L54           50 S L53 SAM SUB=L51
L55       235854 S C5-C6-C6-C6/ES
L56       246303 S L47,L51,L55
L57           50 S L53 SAM SUB=L56
L58               STR L53
L59           50 S L58 SAM SUB=L56
L60        89148 S L58 FUL SUB=L56
L61         1419 S L50 FUL SUB=L60
                SAV L61 QAZI053/A
L62           99 S L60 AND ETHYL CARBON?
L63            1 S L61 AND L62
L64            1 S L61 AND C25H38O6
L65            3 S L61 AND C22H34O4
L66               STR
L67            0 S L66 SAM SUB=L61
L68            8 S L66 FUL SUB=L61
L69            5 S L68 NOT SI/ELS
L70            4 S L69 NOT C27H36O4
L71            1 S L70 AND C25H38O6
L72            3 S L70 NOT L71
L73            2 S L72 NOT C6/ES
L74            3 S L71,L73
                SAV L74 QAZI053A/A

     FILE 'HCAOLD' ENTERED AT 15:31:15 ON 19 AUG 2002
L75            1 S L74
                SEL AN
                EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 15:31:53 ON 19 AUG 2002
L76            2 S E9
L77            1 S L76 NOT CASPI ?/AU
L78            1 S L74

     FILE 'REGISTRY' ENTERED AT 15:32:35 ON 19 AUG 2002

     FILE 'HCAOLD' ENTERED AT 15:33:08 ON 19 AUG 2002

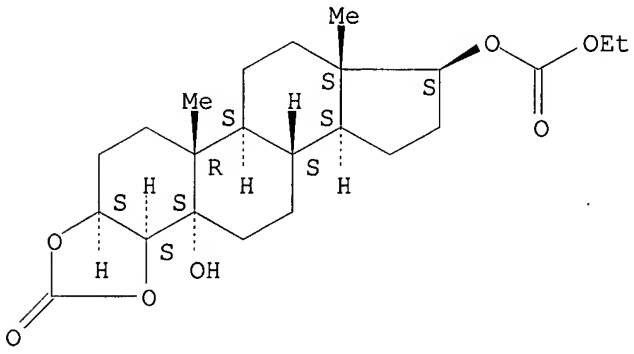
     FILE 'HCAPLUS' ENTERED AT 15:33:14 ON 19 AUG 2002

     FILE 'IFIPAT' ENTERED AT 15:33:36 ON 19 AUG 2002
L79            0 S L74
```

=> d l16 all hitstr

L16 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
AN CA65:18648e CAOLD
TI neighboring-group participation on 3.beta.-acetate, -mixed carbonate, or -urethan groups in acid-catalyzed cleavage of 4.alpha.,5.alpha.-epoxysteroids
AU Julia, Sylvestre; Furer, B.
IT 747-90-0 1156-92-9 1852-61-5 1917-78-8 6564-48-3 10458-44-3
10459-14-0 10459-15-1 10459-16-2 10459-17-3 10459-18-4 10459-19-5
10459-20-8 10459-21-9 10583-86-5 **10583-87-6** 10583-88-7
10583-89-8 10587-46-9 10587-47-0 13001-01-9 13123-29-0 13262-58-3
13289-03-7 13289-04-8 13312-54-4 13381-18-5
IT **10583-87-6**
RN 10583-87-6 CAOLD
CN 5.alpha.-Androstane-3.beta.,4.beta.,5,17.beta.-tetrol, cyclic 3,4-carbonate, 17-(ethyl carbonate) (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.



=>

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **10583-87-6** REGISTRY
CN 5.alpha.-Androstane-3.beta.,4.beta.,5,17.beta.-tetrol, cyclic 3,4-carbonate, 17-(ethyl carbonate) (7CI, 8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H34 O7
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)

Absolute stereochemistry.